

Thermal Transport for Many Body Tight-Binding Models

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We clarify some aspects of the calculation of the thermal transport coefficients. For a tight-binding Hamiltonian we discuss the approximate nature of the charge current and the thermal current obtained by Peierls substitution which is also identical to the equation of motion technique. We address the issue of choosing an appropriate basis for making the Peierls construction for transport calculations. We propose a criteria for finding an optimum Wannier basis where the difference between the exact current and the approximate one is minimum. Using the equations of motion we derive the thermal current for a generalized Hubbard model with density interaction. We identify a part which is the contribution from the long range interactions to the heat current. For the Hubbard model we derive expressions for the transport coefficients in the limit of infinite dimensions.

I. INTRODUCTION

The theoretical description of the thermoelectric response of correlated materials is a fundamental problem in condensed matter physics, and a breakthrough in this area has potential technological useful implications.¹ The materials, which have been studied as likely candidates for useful thermoelectric properties, are mostly semiconductor alloys and compounds. Materials such as $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$ and Si-Ge , which are currently favoured for room temperature application, belong to this category. Another class of materials, with potentially useful thermoelectric properties, are Ce and La filled skutterudites such as $\text{LaFe}_3\text{CoSb}_{12}$ and $\text{CeFe}_3\text{CoSb}_{12}$.¹ Theoretically these materials have been studied successfully using band theory.² Recently Mahan and Sofo³ have shown that the best thermoelectric materials could well be correlated metals and semiconductors (i.e., rare earth intermetallic compounds). The development of the dynamical mean field theory (DMFT)[for reviews see Refs. 4, 5] has allowed new studies of the effects of correlation on the thermoelectric response using this method on model Hamiltonians.^{6,7,8} More recent combinations of band theory and many-body methods such as the LDA+DMFT method⁹ [for reviews see Refs. 10, 11] or the LDA++ method¹² offers the exciting possibility of predicting the thermoelectric properties of materials starting from first principles.¹³ This revival of interest in the thermoelectric response motivates us to re-analyze in this paper the following issues: (1) what is the form of the thermal current and the charge current which should be used in realistic calculations, and (2) how it should be approximated in a DMFT calculation.

The first question is subtle for two reasons. First, as noted early on by Jonson and Mahan,¹⁴ the electronic part of the thermal current operator contains a quadratic and a quartic piece (if the electron-electron interaction is non-local) in the electron creation and annihilation operators. The contribution of this quartic interaction term to the current has continued to be the subject of discussion.¹⁵ Second, while the form of the thermal current and the charge current in the continuum is unambiguous, and

can be calculated using Noether's theorem,^{16,17} DMFT calculations require the projection of these currents on a restricted lattice model. This involves the computation of complicated matrix elements, and in practice an approximation which is analogous to the Peierls substitution¹⁸ for the electrical current is carried out. It is well known that the results of this construction depend on the basis set of orbitals used.¹⁹ This raises the practical question of how to optimize the basis of orbitals to be used in transport calculations.

The second question is subtle due to the presence of interaction terms in the current. This raises the issue of how it should be simplified in the evaluation of the various current-current correlation functions and the transport coefficients. This question was first addressed by Schweitzer and Czycholl²⁰ and by Pruschke and collaborators⁵ who stated that *within the relaxation time approximation*, this term can be expressed in terms of a time derivative, and the vertex corrections can be ignored. In the review of Georges *et. al.*⁴ it was stated that the results of Pruschke *et. al.* hold beyond the relaxation time approximation in the limit of large dimensionality when DMFT becomes exact but no detailed proof of this statement was presented.

The following are our main results. (1) In section II we address the question of the optimization of the basis of localized orbitals for transport calculations, following the ideas of Marzari and Vanderbilt.²¹ For completeness and for pedagogical reasons we discuss in parallel work on the charge current, which is simpler and better understood²² than the thermal current. Our conclusions in this context have applications for the computation of Born charges in empirical tight-binding models.²³ (2) In section III we derive the form of the thermal current to be used in tight-binding models, and its dependence on the orbitals, using the equation of motion technique introduced in Ref. 24. Our final expression differs in one term from the results of Ref. 15. (3) In section IV we describe in detail the diagrammatic analysis of correlation functions of the current operators. We demonstrate explicitly that in the DMFT limit of the transport calculation, the vertex corrections (even for those involving the thermal

current) can be completely neglected, thereby justifying the current practice used in all previous DMFT work.

II. CHARGE CURRENT

We consider a system of electrons in a periodic potential $V(r)$, in the presence of an external vector potential

$\mathbf{A}(r)$, and with coulomb interaction between them. The Lagrangian is given by

$$L = \frac{i}{2} \int d^3r (\psi^\dagger \dot{\psi} - \dot{\psi}^\dagger \psi) + \frac{1}{2m} \int d^3r \psi^\dagger (\nabla - ie\mathbf{A}(r))^2 \psi - \int d^3r V(r) \psi^\dagger \psi - \frac{e^2}{2} \iint d^3r d^3r' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} \psi(\mathbf{r}') \psi(\mathbf{r}). \quad (1)$$

Here $\psi^\dagger(\mathbf{r})$ and $\psi(\mathbf{r})$ are the electron field operators with usual anticommutation properties. We have ignored the spin of the electrons only to simplify the notation. Including spin in the following analysis is quite straightforward. In field theory, when both high and low energy degrees of freedom are retained, Noether's theorem provides a robust procedure to identify the various currents.¹⁷ The theorem associates with every symmetry of the action a conserved charge and a corresponding current. The charge current is determined by the invariance of the action $S = \int dt L(t)$, under $U(1)$ gauge transformation given by $\psi(\mathbf{r}) \rightarrow \psi(\mathbf{r})e^{i\phi(\mathbf{r})}$ and $\psi^\dagger(\mathbf{r}) \rightarrow \psi^\dagger(\mathbf{r})e^{-i\phi(\mathbf{r})}$. The transformation does not produce any variation from

the interaction term, and the well known expression for the charge current is

$$\mathbf{j} = -\frac{ie}{m} \int d^3r \psi^\dagger(\mathbf{r}) (\nabla - ie\mathbf{A}(r)) \psi(\mathbf{r}). \quad (2)$$

The above expression is gauge invariant. The part which is proportional to the vector potential gives the diamagnetic current.

In order to facilitate further discussion we will perform the standard Noether construction in the Wannier basis. In this basis the action (which includes both low and high energy degrees of freedom) is

$$S = \int dt \left\{ \frac{i}{2} \sum_{n\mu} (\dot{c}_n^{\dagger\mu} c_n^\mu - \dot{c}_n^\mu c_n^{\dagger\mu}) - \sum_{nm} t_{nm}^{\mu\nu} c_n^{\dagger\mu} c_m^\nu + \frac{e}{2m} \sum_{nml} \mathbf{p}_{nl}^{\mu\gamma} \cdot \mathbf{A}_{lm}^{\gamma\nu} c_n^{\dagger\mu} c_m^\nu + \frac{e}{2m} \sum_{nml} \mathbf{A}_{nl}^{\mu\gamma} \cdot \mathbf{p}_{lm}^{\gamma\nu} c_n^{\dagger\mu} c_m^\nu - \frac{e^2}{2m} \sum_{nml} \mathbf{A}_{nl}^{\mu\gamma} \cdot \mathbf{A}_{lm}^{\gamma\nu} c_n^{\dagger\mu} c_m^\nu - \frac{1}{2} \sum_{\substack{n_1 \dots n_4 \\ \mu_1 \dots \mu_4}} U_{n_1 \dots n_4}^{\mu_1 \dots \mu_4} c_{n_1}^{\dagger\mu_1} c_{n_2}^{\dagger\mu_2} c_{n_3}^{\mu_3} c_{n_4}^{\mu_4} \right\}, \quad (3)$$

where $t_{nm}^{\mu\nu} = \langle n\mu | \mathcal{H}_0 | m\nu \rangle$, $\mathbf{p}_{nm}^{\mu\nu} = \langle n\mu | \mathbf{p} | m\nu \rangle$, $\mathbf{A}_{nm}^{\mu\nu} = \langle n\mu | \mathbf{A}(r) | m\nu \rangle$, and $U_{n_1 \dots n_4}^{\mu_1 \dots \mu_4} = \langle n_1 \mu_1, n_2 \mu_2 | e^2 / |\mathbf{r} - \mathbf{r}'| | n_4 \mu_4, n_3 \mu_3 \rangle$. Here $\mathcal{H}_0 = \mathbf{p}^2/2m + V(r)$ is the non-interacting part of the Hamiltonian, μ is the band index, and \mathbf{R}_n defines the lattice positions. $W_\mu(\mathbf{r} - \mathbf{R}_n) = \langle \mathbf{r} | n\mu \rangle$ form a complete set of orthonormal Wannier functions. The creation and annihilation operators satisfy the anticommutation relation $\{c_n^\mu, c_m^\nu\} = \delta_{nm} \delta_{\mu\nu}$. The gauge transformation of the fermionic field operators is equivalent to the variation $\delta c_n^\mu = i \int d^3r \phi(\mathbf{r}) \psi(\mathbf{r}) W_\mu^*(\mathbf{r} - \mathbf{R}_n)$ and $\delta c_n^{\dagger\mu} = -i \int d^3r \phi(\mathbf{r}) \psi^\dagger(\mathbf{r}) W_\mu(\mathbf{r} - \mathbf{R}_n)$. Expanding

$\phi(\mathbf{r})$ about the point \mathbf{R}_n and keeping only up to $\nabla\phi$ term (which is all we need to construct the Noether current) we get

$$\begin{aligned} \delta c_n^\mu &= i\phi(\mathbf{R}_n) c_n^\mu + i\nabla\phi \sum_{m\nu} \mathbf{L}_{nm}^{\mu\nu} c_m^\nu, \\ \delta c_n^{\dagger\mu} &= -i\phi(\mathbf{R}_n) c_n^{\dagger\mu} - i\nabla\phi \sum_{m\nu} c_m^{\dagger\nu} \mathbf{L}_{mn}^{\nu\mu}, \end{aligned} \quad (4)$$

where $\mathbf{L}_{nm}^{\mu\nu} = \int d^3r W_\mu^*(\mathbf{r} - \mathbf{R}_n) (\mathbf{r} - \mathbf{R}_n) W_\nu(\mathbf{r} - \mathbf{R}_m)$ are the connection coefficients. The matrix \mathbf{L} is hermitian, i.e., $\mathbf{L}_{nm}^{*\mu\nu} = \mathbf{L}_{mn}^{\nu\mu}$. We note first that the variation from

the interaction term is exactly zero. Next, using the operator identity $[r_i, A_j(r)] = 0$ we find that the variation from the term quadratic in $\mathbf{A}(r)$ is zero. To get the

correct diamagnetic part we make use of $[r_i, p_j] = i\delta_{ij}$. From the invariance of the action we can identify the charge current as

$$\begin{aligned} \mathbf{j} &= ie \sum_{nm} (\mathbf{R}_m - \mathbf{R}_n) t_{nm}^{\mu\nu} c_n^{\dagger\mu} c_m^\nu + ie \sum_{nml} c_n^{\dagger\mu} (t_{nl}^{\mu\gamma} \mathbf{L}_{lm}^{\gamma\nu} - \mathbf{L}_{nl}^{\mu\gamma} t_{lm}^{\gamma\nu}) c_m^\nu - \frac{e^2}{m} \sum_{nm} \mathbf{A}_{nm}^{\mu\nu} c_n^{\dagger\mu} c_m^\nu \\ &= ie \sum_{nm} c_n^{\dagger\mu} c_m^\nu \langle n\mu | [\mathcal{H}_0(\mathbf{A}), \mathbf{r}] | m\nu \rangle. \end{aligned} \quad (5)$$

$\mathcal{H}_0(\mathbf{A}) = (\mathbf{p} - e\mathbf{A})^2/(2m) + V(r)$. This is just equation (2) expressed in the Wannier basis. The charge current is related to the electronic polarization operator²⁵

$$\mathbf{P}_{\text{el}} = e \sum_{nm} c_n^{\dagger\mu} c_m^\nu \langle n\mu | \mathbf{r} | m\nu \rangle$$

by $\partial \mathbf{P}_{\text{el}} / \partial t = \mathbf{j}$. The change in polarization $\Delta \mathbf{P}_{\text{el}}$ (which is a well defined and measurable bulk quantity, rather than polarization itself) between an initial and a final state of a sample is the integrated current flowing through the sample during an adiabatic transformation connecting the two states.²⁶

Theoretical models of the tight-binding type are effective low energy models described in terms of those bands which are close to the Fermi surface.²⁷ The question, which is non-trivial and which is still debated, is what should be the form of the current for such low energy models. The low energy Hamiltonian is obtained by eliminating or integrating out the degrees of freedom corresponding to the high energy bands. This is easily formulated in the functional integral language and the procedure generates many interaction terms that are not present in the original action. In a Hamiltonian formulation this is equivalent to making a canonical transformation to decouple the low energy and the high energy sectors.²⁸ That is, given a full many body Hamiltonian \mathcal{H} , we perform unitary transformation U such that $U\mathcal{H}U^{-1}$ is diagonal (for a system of interacting particles, in general, this can be done only approximately), and then consider only $PU\mathcal{H}U^{-1}P$, where P is the operator projecting on the low energy bands. To obtain the expression for the current in the low energy sector one has to perform the same canonical transformation used to transform the original Hamiltonian into the effective Hamiltonian on the operator representing the current. In other words, we first calculate the current (say, \mathbf{J}) for the full theory

(using the symmetry of the full theory), make the same unitary transformation and then project the current on the low energy sector of interest. The exact low energy current is then given by $PUJU^{-1}P$. This method of calculating the current for the low energy theory is motivated by renormalization group ideas. But, to implement this in practice is usually a formidable task. However, if we consider a system of non-interacting electrons (in a periodic potential) with a subset M of bands that defines the low energy subspace, the low energy current is obtained by projecting the full current in eqn. (5) on the low energy subspace. This is given by $P\mathbf{j}P$, where $P = \sum_{n,\mu \in M} |n\mu\rangle \langle n\mu|$ is the projection operator. We note

that the calculation of the exact current requires knowledge of the matrix elements of the position operator in addition to that of \mathcal{H}_0 (the tight-binding parameters).²⁹

Sometimes, to avoid calculating the matrix elements of the position operator, one makes the approximation known as Peierls substitution. There are two types of approximations involved with this procedure. First, terms involving the connection coefficients are dropped out, and one considers an approximate gauge transformation given by $\delta c_n^\mu = i\phi(\mathbf{R}_n) c_n^\mu$ and $\delta c_n^{\dagger\mu} = -i\phi(\mathbf{R}_n) c_n^{\dagger\mu}$. Putting the connection coefficients to zero is equivalent to the approximation $\langle n\mu | \mathbf{r} | m\nu \rangle \approx \mathbf{R}_n \delta_{nm} \delta_{\mu\nu}$ for the matrix elements of the position operator, and $\langle n\mu | \mathbf{p} | m\nu \rangle = im \langle n\mu | [\mathcal{H}_0, \mathbf{r}] | m\nu \rangle \approx im(\mathbf{R}_m - \mathbf{R}_n) t_{nm}^{\mu\nu}$ for the matrix elements of the momentum operator. Second, with this approximate gauge transformation, the variation from the interaction term is non-zero (though, as already noted, it is zero for the exact gauge transformation). However, contribution to the current from the interaction term is neglected. It will be further assumed that the vector potential is constant, i.e., $\mathbf{A}_{nm}^{\mu\nu} = \mathbf{A} \delta_{nm} \delta_{\mu\nu}$. With these simplifications the approximate current (\mathbf{j}_P) is given by

$$\mathbf{j}_P = ie \sum_{nm} (\mathbf{R}_m - \mathbf{R}_n) t_{nm}^{\mu\nu} c_n^{\dagger\mu} c_m^\nu + e^2 \sum_{nm} (\mathbf{R}_m - \mathbf{R}_n) ((\mathbf{R}_m - \mathbf{R}_n) \cdot \mathbf{A}) t_{nm}^{\mu\nu} c_n^{\dagger\mu} c_m^\nu. \quad (6)$$

The second term is the approximate diamagnetic contribution. The usefulness of \mathbf{j}_P lies in the fact that it can be calculated from the tight-binding parameters alone.

The construction of the Peierls current in terms of the atomic orbitals is *a priori* not obvious for the case when there is more than one atom per unit cell. It is worthwhile to clarify this issue here. We will denote the atomic wavefunctions by $|\alpha\tau\mathbf{R}_n\rangle$, where α is a symmetry index, \mathbf{R}_n is the lattice position of a unit cell, and \mathbf{R}_τ is the position of the atom τ within a unit cell. It is desirable to define the Bloch basis wavefunctions by $|\alpha\tau\mathbf{k}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_n} e^{-i\mathbf{k}\cdot(\mathbf{R}_n+\mathbf{R}_\tau)} |\alpha\tau\mathbf{R}_n\rangle$, though the phase factor $e^{-i\mathbf{k}\cdot\mathbf{R}_\tau}$ is quite innocuous for the definition of the Hamiltonian matrix $\mathcal{H}(\mathbf{k})_{\alpha_1\tau_1;\alpha_2\tau_2}$ and for the subsequent calculation of the energy bands. The question, whether to keep the phase factor or not, is however important for the definition of the Peierls current $\mathbf{j}_P(\mathbf{k})_{\alpha_1\tau_1;\alpha_2\tau_2} = \frac{\partial}{\partial \mathbf{k}} \mathcal{H}(\mathbf{k})_{\alpha_1\tau_1;\alpha_2\tau_2}$. It is easy to verify that, with the above definition of the Bloch basis, one gets the same form for the Peierls current if one considers a lattice with one atom per unit cell (for which case the definition of the Peierls current is unambiguous), and

compare it with the same lattice with its period doubled (and therefore now with two identical atoms per unit cell).

We will examine the behaviour of the exact current and the approximate one under infinitesimal unitary transformation $U_{nm}^{\mu\nu} = \delta_{nm}\delta_{\mu\nu} + W_{nm}^{\mu\nu}$ (where W is antihermitian) of the Wannier functions defined by $|n\mu\rangle \rightarrow \sum_{m\nu} U_{mn}^{\nu\mu} |m\nu\rangle$. The variation of a matrix element $(\mathbf{j})_{nm}^{\mu\nu} = ie\langle n\mu | [\mathcal{H}_0(\mathbf{A}), \mathbf{r}] | m\nu \rangle$ of the exact current is given by

$$(\mathbf{j})_{nm}^{\mu\nu} \rightarrow (\mathbf{j})_{nm}^{\mu\nu} + \sum_{k,\gamma} \{ (\mathbf{j})_{nk}^{\mu\gamma} W_{km}^{\gamma\nu} - W_{nk}^{\mu\gamma} (\mathbf{j})_{km}^{\gamma\nu} \}. \quad (7)$$

This is the usual transformation of matrix elements of operators that remain invariant under unitary transformation. In fact, the paramagnetic and the diamagnetic parts of the operator \mathbf{j} are separately invariant. The behaviour of \mathbf{j}_P is however different. The variation of $(\mathbf{j}_P)_{nm}^{\mu\nu} = ie(\mathbf{R}_m - \mathbf{R}_n)t_{nm}^{\mu\nu} + e^2(\mathbf{R}_m - \mathbf{R}_n)((\mathbf{R}_m - \mathbf{R}_n) \cdot \mathbf{A})t_{nm}^{\mu\nu}$ is given by

$$\begin{aligned} (\mathbf{j}_P)_{nm}^{\mu\nu} \rightarrow & (\mathbf{j}_P)_{nm}^{\mu\nu} + \sum_{k,\gamma} \{ (\mathbf{j}_P)_{nk}^{\mu\gamma} W_{km}^{\gamma\nu} - W_{nk}^{\mu\gamma} (\mathbf{j}_P)_{km}^{\gamma\nu} \} + ie \sum_{k,\gamma} (\mathbf{R}_m - \mathbf{R}_k) t_{nk}^{\mu\gamma} W_{km}^{\gamma\nu} - ie \sum_{k,\gamma} (\mathbf{R}_k - \mathbf{R}_n) W_{nk}^{\mu\gamma} t_{km}^{\gamma\nu} \\ & + e^2 \sum_{k,\gamma} \{ (\mathbf{R}_k - \mathbf{R}_n) ((\mathbf{R}_m - \mathbf{R}_k) \cdot \mathbf{A}) + (\mathbf{R}_m - \mathbf{R}_k) ((\mathbf{R}_m - \mathbf{R}_n) \cdot \mathbf{A}) \} t_{nk}^{\mu\gamma} W_{km}^{\gamma\nu} \\ & - e^2 \sum_{k,\gamma} \{ (\mathbf{R}_m - \mathbf{R}_k) ((\mathbf{R}_k - \mathbf{R}_n) \cdot \mathbf{A}) + (\mathbf{R}_k - \mathbf{R}_n) ((\mathbf{R}_m - \mathbf{R}_n) \cdot \mathbf{A}) \} W_{nk}^{\mu\gamma} t_{km}^{\gamma\nu}. \end{aligned} \quad (8)$$

The paramagnetic and the diamagnetic parts of \mathbf{j}_P are both basis dependent operators.

The basis dependence of \mathbf{j}_P raises the practical question as to what basis one should choose while making the Peierls construction. For example, there have been efforts to calculate polarization properties, like effective charges of semiconductors, using the empirical tight-binding theory.²³ In this scheme a natural approximation is the “diagonal” ansatz which assumes that the position operator is diagonal in the tight-binding basis with expectation values equal to the atomic positions. This is equivalent to a Peierls substitution, and the polarization calculated with this ansatz is related to Peierls current \mathbf{j}_P . The effective charges calculated in this procedure depends on the choice of the underlying Wannier basis. In order to improve the results one should first make an appropriate choice of a basis. One possibility is to use the basis of the “maximally localized” Wannier functions that was introduced by Marzari and Vanderbilt.²¹ This is obtained by minimizing a functional which measures the spread of the Wannier functions. Intuitively, it seems plausible that the approximation in which the connec-

tion coefficients are neglected, will work better in a basis where the Wannier functions are more localized. A second possibility, suggested by Millis,¹⁹ is to choose that basis in which the charge stiffness calculated using the Peierls current will be closest to the one obtained from band theory. We note that this criteria is already satisfied by the Bloch basis in which the effective one-electron Hamiltonian is diagonal in the band indices. This can be seen easily in the following manner. We consider the scenario of band theory where electrons are in an effective periodic potential. Let $\epsilon_{\mathbf{k}\mu}$ denote the single particle energy levels. It can be shown that the charge stiffness is given by $D_{\alpha\beta} = \sum_{\mathbf{k}\mu} f(\epsilon_{\mathbf{k}\mu}) (\partial^2 \epsilon_{\mathbf{k}\mu} / (\partial k_\alpha \partial k_\beta))$.³⁰ Here $f(\epsilon)$ is the Fermi function and α, β denote spatial directions. The Peierls current constructed in the Bloch basis does not have any interband term since the basis is already diagonal in the band indices. The paramagnetic part of the current is given by $(j_P)_{\text{para},\alpha} = \sum_{\mathbf{k}\mu} (\partial \epsilon_{\mathbf{k}\mu} / \partial k_\alpha) c_{\mathbf{k}}^{\dagger\mu} c_{\mathbf{k}}^\mu$. Since the paramagnetic part has no interband matrix element, it does not contribute to the charge stiffness. The diamagnetic part, given by $(j_P)_{\text{dia},\alpha} = - \sum_{\mathbf{k}\mu\beta} (\partial^2 \epsilon_{\mathbf{k}\mu} / (\partial k_\alpha \partial k_\beta)) A_{\beta} c_{\mathbf{k}}^{\dagger\mu} c_{\mathbf{k}}^\mu$, gives a

charge stiffness exactly equal to that obtained from band theory. It is possible, though, that there are other bases which satisfy this criteria.

In passing we note that if the matrix elements of the exact current \mathbf{j} are known by some means, say, from first principles calculation, then it is possible to define the functional

$$\Omega = \sum_{\substack{nm \\ \mu\nu \in M}} \langle n\mu | \mathbf{j} - \mathbf{j}_P | m\nu \rangle \cdot \langle m\nu | \mathbf{j} - \mathbf{j}_P | n\mu \rangle \quad (9)$$

$$\begin{aligned} G_{nm}^{\mu\nu} = & (\mathbf{R}_m - \mathbf{R}_n) \cdot \langle n\mu | [\mathcal{H}_0, (\mathbf{j} - \mathbf{j}_P)] | m\nu \rangle + ie ((\mathbf{R}_m \cdot \mathbf{A})\mathbf{R}_m - (\mathbf{R}_n \cdot \mathbf{A})\mathbf{R}_n) \cdot \langle n\mu | \{\mathcal{H}_0, (\mathbf{j} - \mathbf{j}_P)\} | m\nu \rangle \\ & - ie \sum_{k\gamma} \{ (\mathbf{R}_m - \mathbf{R}_n)(\mathbf{R}_k \cdot \mathbf{A}) + ((\mathbf{R}_m - \mathbf{R}_n) \cdot \mathbf{A})\mathbf{R}_k \} \\ & \cdot \{ \langle n\mu | \mathbf{j} - \mathbf{j}_P | k\gamma \rangle \langle k\gamma | \mathcal{H}_0 | m\nu \rangle + \langle n\mu | \mathcal{H}_0 | k\gamma \rangle \langle k\gamma | \mathbf{j} - \mathbf{j}_P | m\nu \rangle \} \end{aligned} \quad (10)$$

The optimum basis is the one for which the gradient vanishes. The choice of basis will depend on the vector potential, but the physical quantities calculated in that basis will not. In general, this criteria will give a basis which is different from that of the “maximally localized” Wannier functions. The above method of choosing an appropriate basis is not very useful for doing charge transport calculations because to define the method one needs to know the matrix elements of the exact current, knowing which makes the Peierls construction redundant. However, one can use this optimization procedure for doing thermal transport calculation. As we will see in the next section, the matrix elements of the exact thermal current are quite complicated, and a Peierls formulation of the thermal current is desirable (in some suitable basis). The rationale for our suggestion is that the basis which

and choose the basis which minimizes Ω , and thereby the difference between the exact current and the approximate one. Using eqns. [7] and [8] we can calculate the variation of Ω under infinitesimal unitary transformation. The gradient, defined as $G_{nm}^{\mu\nu} = d\Omega/dW_{nm}^{\mu\nu}$, is given by

optimizes the Peierls construction for electric transport will be a good basis for doing the Peierls construction for thermal transport as well.

III. THERMAL CURRENT

In field theory the energy current (which is same as the thermal current, except for the latter the single particle energies are measured from the chemical potential) is determined from the invariance of the action under the transformation of time $t \rightarrow t - \phi(\mathbf{r}, t)$. This shifts the field operators by $\delta\psi = \dot{\psi}\phi$, and $\delta\psi^\dagger = \dot{\psi}^\dagger\phi$. From the variation of the action defined in equation (1), the energy current (\mathbf{j}_E) is given by

$$\begin{aligned} \mathbf{j}_E = & -\frac{1}{2m} \int d^4r \left\{ \dot{\psi}^\dagger \nabla \psi + \nabla \psi^\dagger \dot{\psi} \right\} + \frac{1}{4} \int d^3\mathbf{r}_1 \int d^3\mathbf{r}_2 (\mathbf{r}_2 - \mathbf{r}_1) \\ & U(r_1 - r_2) \left\{ \dot{\psi}^\dagger(\mathbf{r}_1) \rho(\mathbf{r}_2) \psi(\mathbf{r}_1) - \psi^\dagger(\mathbf{r}_1) \dot{\rho}(\mathbf{r}_2) \psi(\mathbf{r}_1) + \psi^\dagger(\mathbf{r}_1) \rho(\mathbf{r}_2) \dot{\psi}(\mathbf{r}_1) \right\}. \end{aligned} \quad (11)$$

Here $\rho(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r})$, and $U(r)$ is the two-particle interaction energy (Coulomb potential, in our case). The second term above, which is formally quartic in the field operators, is the contribution to energy current from the non-local (in space) interaction. This term was missed by Langer,¹⁶ but noted in a different context by Jonson and Mahan.¹⁴ More recently, it has been discussed by Moreno and Coleman.¹⁵

We have discussed in the previous section that for an effective low-energy model any current is obtained correctly by projecting the current for the full theory

(where both high and low energy degrees of freedom are present) on the low-energy bands. To implement this for the energy current one has to consider variations of the Wannier operators $\delta c_i^\mu = \phi(\mathbf{R}_i) \dot{c}_i^\mu + \nabla\phi \sum_{j,\nu} \mathbf{L}_{ij}^{\mu\nu} \dot{c}_j^\nu$ and $\delta c_i^{\dagger\mu} = \phi(\mathbf{R}_i) \dot{c}_i^{\dagger\mu} + \nabla\phi \sum_{j,\nu} \dot{c}_j^{\dagger\nu} \mathbf{L}_{ji}^{\nu\mu}$ under translation of time. If we ignore the terms with the connection coefficients, we get an approximate current which is equivalent to a Peierls substitution. The same approximate current can be derived from the low-energy effective Hamiltonian using the equations of motion.²⁴ Although we are emphasizing the importance of the exact low-energy current, in

practice, calculating the exact thermal current is fairly complicated. Therefore, we will restrict the derivation to that of a Peierls type of energy current for a generalized Hubbard model described by the Hamiltonian

$$\mathcal{H} = \sum_{ij}^{\mu\nu, \sigma} t_{ij}^{\mu\nu} c_{i\sigma}^{\dagger\mu} c_{j\sigma}^{\nu} + \sum_{ij}^{\mu\nu, \sigma\sigma'} V_{ij, \sigma\sigma'}^{\mu\nu} n_{i\sigma}^{\mu} n_{j\sigma'}^{\nu}, \quad (12)$$

using the equation of motion technique. Here $n_{i\sigma}^{\mu} = c_{i\sigma}^{\dagger\mu} c_{i\sigma}^{\mu}$. The local energy density (h_i) is given by

$$h_i = \frac{1}{2} \sum_{j}^{\mu\nu, \sigma} \left(t_{ij}^{\mu\nu} c_{i\sigma}^{\dagger\mu} c_{j\sigma}^{\nu} + t_{ji}^{\nu\mu} c_{j\sigma}^{\dagger\nu} c_{i\sigma}^{\mu} \right)$$

It can be shown that

$$\begin{aligned} \dot{h}_i = & \frac{1}{2} \sum_{j}^{\mu\nu, \sigma} \left\{ t_{ij}^{\mu\nu} \left(c_{i\sigma}^{\dagger\mu} \dot{c}_{j\sigma}^{\nu} - \dot{c}_{i\sigma}^{\dagger\mu} c_{j\sigma}^{\nu} \right) + t_{ji}^{\nu\mu} \left(\dot{c}_{j\sigma}^{\dagger\nu} c_{i\sigma}^{\mu} - c_{j\sigma}^{\dagger\nu} \dot{c}_{i\sigma}^{\mu} \right) \right\} \\ & + \frac{1}{2} \sum_{j}^{\mu\nu, \sigma\sigma'} V_{ij, \sigma\sigma'}^{\mu\nu} \left(-\dot{c}_{i\sigma}^{\dagger\mu} c_{j\sigma'}^{\dagger\nu} c_{j\sigma'}^{\nu} c_{i\sigma}^{\mu} + c_{i\sigma}^{\dagger\mu} \dot{c}_{j\sigma'}^{\dagger\nu} c_{j\sigma'}^{\nu} c_{i\sigma}^{\mu} + c_{i\sigma}^{\dagger\mu} c_{j\sigma'}^{\dagger\nu} \dot{c}_{j\sigma'}^{\nu} c_{i\sigma}^{\mu} - c_{i\sigma}^{\dagger\mu} c_{j\sigma'}^{\dagger\nu} c_{j\sigma'}^{\nu} \dot{c}_{i\sigma}^{\mu} \right) \\ & + \frac{1}{2} \sum_{j}^{\mu\nu, \sigma\sigma'} V_{ji, \sigma'\sigma}^{\nu\mu} \left(\dot{c}_{j\sigma'}^{\dagger\nu} c_{i\sigma}^{\dagger\mu} c_{i\sigma}^{\nu} c_{j\sigma'}^{\mu} - c_{j\sigma'}^{\dagger\nu} \dot{c}_{i\sigma}^{\dagger\mu} c_{i\sigma}^{\nu} c_{j\sigma'}^{\mu} - c_{j\sigma'}^{\dagger\nu} c_{i\sigma}^{\dagger\mu} \dot{c}_{i\sigma}^{\nu} c_{j\sigma'}^{\mu} + c_{j\sigma'}^{\dagger\nu} c_{i\sigma}^{\dagger\mu} c_{i\sigma}^{\nu} \dot{c}_{j\sigma'}^{\mu} \right), \end{aligned} \quad (13)$$

where $\dot{O} = i[\mathcal{H}, \hat{O}]$. The energy current (\mathbf{j}_E) is related to the energy density by the continuity equation $\dot{h}_i + \nabla \cdot \mathbf{j}_E(i) = 0$. We define $h(\mathbf{q}) = \sum_i e^{-i\mathbf{q} \cdot \mathbf{R}_i} h_i$, and similarly $\mathbf{j}_E(\mathbf{q})$. The Fourier transform of the Wannier operators are defined by $c_{\mathbf{k}\sigma}^{\mu} = \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{k} \cdot \mathbf{R}_i} c_{i\sigma}^{\mu}$, and similarly for $c_{\mathbf{k}\sigma}^{\dagger\mu}$. Here N is the size of the lattice. Comparing with the continuity equation we get the energy current

$$\begin{aligned} \mathbf{j}_E = & \frac{i}{2} \sum_{\mathbf{k}}^{\mu\nu, \sigma} \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}}^{\mu\nu} \left(c_{\mathbf{k}, \sigma}^{\dagger\mu} \dot{c}_{\mathbf{k}, \sigma}^{\nu} - \dot{c}_{\mathbf{k}, \sigma}^{\dagger\mu} c_{\mathbf{k}, \sigma}^{\nu} \right) \\ & + \frac{i}{2} \sum_{\mathbf{k}\mathbf{k}'}^{\mu\nu, \sigma\sigma'} \nabla_{\mathbf{k}} V_{\mathbf{k}, \sigma\sigma'}^{\mu\nu} \left(c_{\mathbf{k}', \sigma}^{\dagger\mu} \dot{n}_{\mathbf{k}, \sigma'}^{\nu} c_{\mathbf{k}' - \mathbf{k}, \sigma}^{\mu} \right. \\ & \left. - \dot{c}_{\mathbf{k}', \sigma}^{\dagger\mu} n_{\mathbf{k}, \sigma'}^{\nu} c_{\mathbf{k}' - \mathbf{k}, \sigma}^{\mu} - c_{\mathbf{k}', \sigma}^{\dagger\mu} n_{\mathbf{k}, \sigma'}^{\nu} \dot{c}_{\mathbf{k}' - \mathbf{k}, \sigma}^{\mu} \right), \end{aligned} \quad (14)$$

where $n_{\mathbf{k}, \sigma}^{\mu} = \sum_{\mathbf{k}'} c_{\mathbf{k}', \sigma}^{\dagger\mu} c_{\mathbf{k}' + \mathbf{k}, \sigma}^{\mu}$. The first two terms (the quadratic part) in the above eqn. are contributions to the energy current from the electron hopping and from the local part of the interactions. The last three terms (the quartic part) are additional contributions to energy flow from the long range interactions. Moreno and Coleman¹⁵ have calculated the quartic part using Noether's theorem for classical fields, and their result is $\frac{i}{2} \sum_{\mathbf{k}, \mu\nu, \sigma\sigma'} \nabla_{\mathbf{k}} V_{\mathbf{k}, \sigma\sigma'}^{\mu\nu} \left(n_{-\mathbf{k}, \sigma}^{\mu} \dot{n}_{\mathbf{k}, \sigma'}^{\nu} - \dot{n}_{-\mathbf{k}, \sigma}^{\mu} n_{\mathbf{k}, \sigma'}^{\nu} \right)$. We want to argue that this result is incorrect. We note that

$$+ \frac{1}{2} \sum_{j}^{\mu\nu, \sigma\sigma'} \left(V_{ij, \sigma\sigma'}^{\mu\nu} n_{i\sigma}^{\mu} n_{j\sigma'}^{\nu} + V_{ji, \sigma'\sigma}^{\nu\mu} n_{j\sigma'}^{\nu} n_{i\sigma}^{\mu} \right).$$

for classical fields the issue of correct arrangement of operators is not present. Indeed, if we could commute the third operator with the second in each of the last three terms of eqn. (14) we would get the result derived in Ref. (15). However such commutation will generate an additional term $\sum_{\mathbf{k}\mathbf{k}', \mu\nu, \sigma} \nabla_{\mathbf{k}} V_{\mathbf{k}, \sigma\sigma'}^{\mu\nu} \epsilon_{\mathbf{k}' - \mathbf{k}}^{\mu\nu} c_{\mathbf{k}', \sigma}^{\dagger\mu} c_{\mathbf{k}, \sigma}^{\nu}$. Thus, proper

arrangement of operators is important to get the correct form of the energy current, which is naturally captured in an equation of motion technique but not while using Noether's theorem for classical fields.

The heat current (\mathbf{j}_Q) is related to the energy current by $\mathbf{j}_Q = \mathbf{j}_E - \mu \mathbf{j}$, where μ is the chemical potential.²⁴ The chemical potential enters only to shift the single particle energies, i.e., right hand side of eqn. (14) gives the heat current with the re-definition $\dot{O} = i[\mathcal{H} - \mu \mathcal{N}, \hat{O}]$, where \mathcal{N} is the total particle operator.

IV. TRANSPORT COEFFICIENTS

In this section we will examine in detail the derivation of the correlation functions of the current operators. We will consider only the Peierls type of (charge and thermal) currents to keep things analytically tractable. In Kubo formalism the correlation functions are related to the corresponding response functions (the transport coefficients). In the framework of DMFT⁴ it is possible

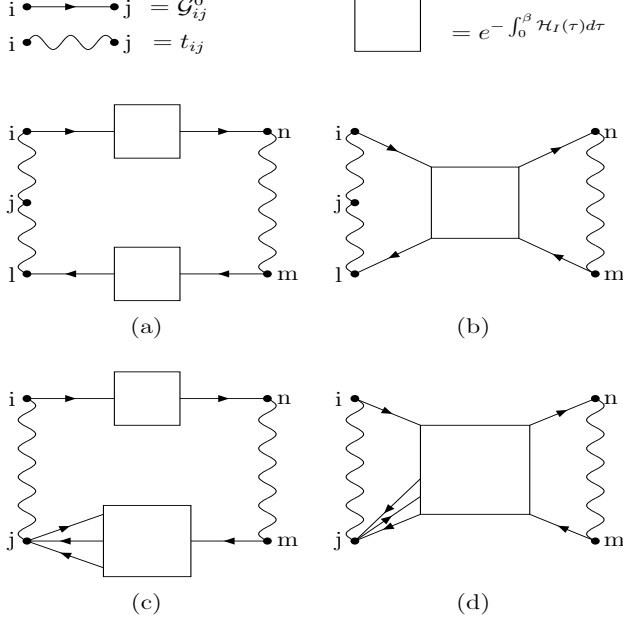


FIG. 1: Diagrams in configuration space for thermoelectric power. \mathcal{H}_I is the interaction term. In (a) and (b) the thermal current is a two-point vertex, while in (c) and (d) it is a four-point vertex. In the limit of infinite d contribution from (b) and (d) can be neglected.

to derive exact expressions for the transport coefficients. The essential simplification in the limit of infinite dimensions (d) is that the self energy and the vertex terms are local. For the single-band Hubbard model, defined by the Hamiltonian

$$\mathcal{H} = \sum_{\langle ij \rangle, \sigma} \left(t_{ij} c_{i, \sigma}^\dagger c_{j, \sigma} + \text{h.c.} \right) + U \sum_i n_{i, \uparrow} n_{i, \downarrow},$$

we will demonstrate that this allows the correlation functions to be factorized into products of single particle Green's functions and their time derivatives. The terms that are ignored by such factorization are $\mathcal{O}(1/d)$ smaller and can be neglected in the limit of infinite d . Using a slightly different approach, the expressions for the transport coefficients for the Falikov-Kimball model have been derived recently.⁸

The correlation functions of the current operators are defined as²⁴

$$L_{ab}(i\omega_n) = \frac{1}{\beta i\omega_n V} \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau \mathbf{j}_a(\tau) \mathbf{j}_b(0) \rangle, \quad (15)$$

where $a, b = (1, 2)$, and $\mathbf{j}_1 = \mathbf{j}$ is the charge current and $\mathbf{j}_2 = \mathbf{j}_Q$ is the heat current. Here V is the volume of the system, $\beta = 1/k_B T$ is inverse temperature, and $i\omega_n$ is bosonic Matsubara frequency. The transport coefficients (that enter the formula for DC conductivity, thermoelectric power and thermal conductivity) are given by,

$$L_{ab} = \lim_{\omega \rightarrow 0} \text{Im} L_{ab}(i\omega_n \rightarrow \omega + i\delta). \quad (16)$$

For the single band Hubbard model the charge current is given by,

$$\mathbf{j} = e \sum_{\mathbf{k}, \sigma} \mathbf{v}_{\mathbf{k}} c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} = e \sum_{\langle ij \rangle, \sigma} i(\mathbf{R}_j - \mathbf{R}_i) t_{ij} c_{i, \sigma}^\dagger c_{j, \sigma}, \quad (17)$$

and the heat current is given by

$$\begin{aligned} \mathbf{j}_Q &= \frac{i}{2} \sum_{\mathbf{k}, \sigma} \mathbf{v}_{\mathbf{k}} \left(c_{\mathbf{k}, \sigma}^\dagger \dot{c}_{\mathbf{k}, \sigma} - \dot{c}_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} \right) \\ &= \frac{1}{2} \sum_{\langle ij \rangle, \sigma} (\mathbf{R}_i - \mathbf{R}_j) t_{ij} \left(c_{i, \sigma}^\dagger \dot{c}_{j, \sigma} - \dot{c}_{i, \sigma}^\dagger c_{j, \sigma} \right). \end{aligned} \quad (18)$$

Here $\mathbf{v}_{\mathbf{k}} = \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}}$ is the electron velocity. Since the interaction is purely local, there is no contribution from the long range interactions.

The derivation of L_{11} is discussed extensively in the literature on DMFT^{5,20} In infinite d the particle-hole vertex becomes momentum independent,³¹ and the dressed correlation function becomes equal to the bare one. This implies the correlation function can be factorized into a product of single particle Green's functions, i.e., $\langle T_\tau \mathbf{j}(\tau) \mathbf{j}(0) \rangle = -\frac{e^2}{d} \sum_{\mathbf{k}, \sigma} v_{\mathbf{k}}^2 \mathcal{G}_\sigma(\mathbf{k}, \tau) \mathcal{G}_\sigma(\mathbf{k}, -\tau)$, where $\mathcal{G}_\sigma(\mathbf{k}, \tau) = -\langle T_\tau c_{\mathbf{k}, \sigma}(\tau) c_{\mathbf{k}, \sigma}^\dagger(0) \rangle$ is the fermionic Matsubara Green's function. We define the Fourier transform $\mathcal{G}_\sigma(\mathbf{k}, \tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} \mathcal{G}_\sigma(\mathbf{k}, i\omega_n)$, in terms of which

$$\begin{aligned} L_{11}(i\omega_n) &= \\ &= -\left(\frac{e^2}{\beta i\omega_n d V} \right) \sum_{\mathbf{k}, \sigma, ip_n} v_{\mathbf{k}}^2 \frac{1}{\beta} \mathcal{G}_\sigma(\mathbf{k}, i\omega_n + ip_n) \mathcal{G}_\sigma(\mathbf{k}, ip_n). \end{aligned}$$

$\mathcal{G}_\sigma(\mathbf{k}, z)$ has a possible branch cut at $z = \epsilon$ and $\mathcal{G}_\sigma(\mathbf{k}, z + i\omega_n)$ has one at $z = \epsilon - i\omega_n$.²⁴ Following Mahan^{14,24} one can show

$$\begin{aligned} \frac{1}{\beta} \sum_{ip_n} \mathcal{G}_\sigma(\mathbf{k}, i\omega_n + ip_n) \mathcal{G}_\sigma(\mathbf{k}, ip_n) &= \\ &= \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} n_F(\epsilon) A_\sigma(\mathbf{k}, \epsilon) [\mathcal{G}_\sigma(\mathbf{k}, \epsilon + i\omega_n) + \mathcal{G}_\sigma(\mathbf{k}, \epsilon - i\omega_n)], \end{aligned}$$

where $A_\sigma(\mathbf{k}, \epsilon) = -2\text{Im} G_\sigma^R(\mathbf{k}, \epsilon)$ is the spectral function and $n_F(\epsilon)$ is the Fermi function. After analytic continuation $i\omega_n \rightarrow \omega + i\delta$, and after taking the static limit we get

$$L_{11} = \frac{e^2}{2d\beta V} \sum_{\mathbf{k}, \sigma} v_{\mathbf{k}}^2 \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \left(-\frac{\partial n_F(\epsilon)}{\partial \epsilon} \right) A_\sigma^2(\mathbf{k}, \epsilon). \quad (19)$$

The derivation of L_{21} is more involved, and is not well discussed in the literature. Since the heat current has a part which is a four-point vertex, *a priori* it is not clear whether a factorization of the correlation function into products of single particle Green's functions and their time derivatives is possible. We have

$\dot{c}_{i,\sigma} = -i \sum_l t_{il} c_{l,\sigma} - iU c_{i,\sigma} n_{i,\bar{\sigma}} + i\mu c_{i,\sigma}$ (and similarly for $\dot{c}_{i,\sigma}^\dagger$). We ignore the term with the chemical potential for the time being (the result remains unchanged). Due to the first term the heat current is a two-point vertex, and the corresponding diagrams for L_{21} are of the type (a) and (b) of Fig. 1. The heat current is a four-point vertex due to the second term. The corresponding diagrams are of the type (c) and (d) of Fig. 1. In the limit of infinite d the scaling of the hopping term is $t_{ij} = t_{ij}^*/\sqrt{d}$ (Ref. 4). This implies that $\mathcal{G}_{ij}^0 \sim (1/\sqrt{d})^{|i-j|}$ (Ref. 4). One can show explicitly that diagrams (a) and (c) are $\mathcal{O}(1/d)$ (and higher), and diagrams (b) and (d) are $\mathcal{O}(1/d^2)$ (and

higher). In Fig.1, $\mathcal{H}_I = U \sum_i n_{i,\uparrow} n_{i,\downarrow}$ is the interaction term of the Hubbard Hamiltonian. In the limit of infinite d the latter drops out, and the factorization of the correlation function is possible. In imaginary time

$$\langle T_\tau \mathbf{j}_Q(\tau) \mathbf{j}(0) \rangle \stackrel{d \rightarrow \infty}{=} \frac{e}{2d} \sum_{\mathbf{k}, \sigma} v_{\mathbf{k}}^2 \left\{ \langle T_\tau \dot{c}_{\mathbf{k},\sigma}(\tau) c_{\mathbf{k},\sigma}^\dagger(0) \rangle \langle T_\tau c_{\mathbf{k},\sigma}(0) c_{\mathbf{k},\sigma}^\dagger(\tau) \rangle + \text{h.c.} \right\}.$$

Using $\frac{\partial}{\partial \tau} \mathcal{G}(\tau) = \langle T_\tau \frac{\partial}{\partial \tau} c(\tau) c^\dagger(0) \rangle - \delta(\tau)$ (in imaginary time), we get

$$L_{21}(i\omega_n) = - \left(\frac{e}{d} \right) \left(\frac{1}{\beta i \omega_n V} \right) \sum_{\mathbf{k}, \sigma} v_{\mathbf{k}}^2 \left\{ \frac{1}{\beta} \sum_{ip_n} \left(ip_n + \frac{i\omega_n}{2} \right) \mathcal{G}_\sigma(\mathbf{k}, ip_n) \mathcal{G}_\sigma(\mathbf{k}, ip_n + i\omega_n) - n_{\mathbf{k},\sigma} \right\}.$$

We drop the second term within braces because it does not contribute to $\text{Im} L_{21}(\omega + i\delta)$. The rest is evaluated like $L_{11}(i\omega_n)$. It can be shown that

$$\begin{aligned} \frac{1}{\beta} \sum_{ip_n} \left(ip_n + \frac{i\omega_n}{2} \right) \mathcal{G}_\sigma(\mathbf{k}, ip_n) \mathcal{G}_\sigma(\mathbf{k}, ip_n + i\omega_n) = \\ \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} n_F(\epsilon) A_\sigma(\mathbf{k}, \epsilon) \left[\left(\epsilon + \frac{i\omega_n}{2} \right) \mathcal{G}_\sigma(\mathbf{k}, \epsilon + i\omega_n) \right. \\ \left. + \left(\epsilon - \frac{i\omega_n}{2} \right) \mathcal{G}_\sigma(\mathbf{k}, \epsilon - i\omega_n) \right]. \end{aligned}$$

After analytic continuation and taking the static limit we get,

$$L_{21} = \frac{e}{2d\beta V} \sum_{\mathbf{k}, \sigma} v_{\mathbf{k}}^2 \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \epsilon \left(-\frac{\partial n_F(\epsilon)}{\partial \epsilon} \right) A_\sigma^2(\mathbf{k}, \epsilon). \quad (20)$$

The derivation of L_{22} is analogous to that of L_{21} . In the limit of infinite d , $\langle T_\tau \mathbf{j}_Q(\tau) \mathbf{j}_Q \rangle$ factorizes into products of (imaginary) time derivatives of single particle Green's functions (plus terms which do not contribute to $\text{Im} L_{22}(\omega)$). As in the case of L_{11} and L_{21} , the terms which are dropped out by such factorization are at least $\mathcal{O}(1/d)$ smaller. In other words,

$$\begin{aligned} \langle T_\tau \mathbf{j}_Q(\tau) \mathbf{j}_Q \rangle \stackrel{d \rightarrow \infty}{=} \frac{1}{4d} \sum_{\mathbf{k}, \sigma} v_{\mathbf{k}}^2 \left\{ \langle T_\tau \dot{c}_{\mathbf{k},\sigma}(\tau) c_{\mathbf{k},\sigma}^\dagger(0) \rangle \langle T_\tau c_{\mathbf{k},\sigma}(0) \dot{c}_{\mathbf{k},\sigma}^\dagger(\tau) \rangle \right. \\ \left. - \langle T_\tau \ddot{c}_{\mathbf{k},\sigma}(\tau) c_{\mathbf{k},\sigma}^\dagger(0) \rangle \langle T_\tau c_{\mathbf{k},\sigma}(0) c_{\mathbf{k},\sigma}^\dagger(\tau) \rangle + \text{h.c.} \right\}. \end{aligned}$$

With this simplification it can be shown that

$$L_{22}(i\omega_n) = - \left(\frac{1}{d} \right) \left(\frac{1}{\beta i \omega_n V} \right) \sum_{\mathbf{k}, \sigma} v_{\mathbf{k}}^2 \left\{ \frac{1}{\beta} \sum_{ip_n} \left(ip_n + \frac{i\omega_n}{2} \right)^2 \mathcal{G}_\sigma(\mathbf{k}, ip_n) \mathcal{G}_\sigma(\mathbf{k}, ip_n + i\omega_n) + \dots \right\}.$$

The terms in the ellipses do not contribute to $\text{Im} L_{22}(\omega)$. Finally we get,

$$L_{22} = \frac{e}{2d\beta V} \sum_{\mathbf{k}, \sigma} v_{\mathbf{k}}^2 \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \epsilon^2 \left(-\frac{\partial n_F(\epsilon)}{\partial \epsilon} \right) A_\sigma^2(\mathbf{k}, \epsilon). \quad (21)$$

We reiterate the observation made in Ref. (8) that the above expressions for the transport coefficients are correct for any model with local interaction (for which Eq.

[18] is correct), in infinite dimensions.

V. CONCLUSION

The current (charge or thermal) obtained by Peierls substitution or by the equation of motion technique is an approximation to the exact low energy current for an effective tight-binding Hamiltonian. In particular, the ap-

proximate current is not invariant under a unitary transformation of the Wannier basis. We have suggested a simple criteria by which one can choose a set of Wannier functions where the difference between the exact and the approximate current is minimum. The minimization procedure is well defined provided the matrix elements of the exact current are known from first principles calculation. Using the equations of motion we have derived the thermal current for a very general tight-binding Hamiltonian, correcting the result of a previous work. Finally, using the Peierls currents, we have established the correctness of known expressions for the transport coefficients for the Hubbard model in infinite d . The simplification in the limit of large coordination is that the current (charge

and thermal) correlation functions can be factorized into products of single particle Green's functions and their time derivatives. These expressions are correct for any model with local interaction and in infinite dimensions.

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